

ENDF Format Manual

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NNDC – BNL

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Overview

- Motivation
- Achievements
- Maintenance
- Status

Motivation

- Manual has been “converted” into different word-processors several times
- In the process, typing errors were accumulated, rather than removed
- The form and layout were particularly difficult to maintain (equations, cross-references, etc.)
(*what you see is what you get – maybe*)
- → Convert once more into LaTeX

Achievements

- Conversion into LaTeX was completed
- Automatic conversion helped, but was poor with equations
- The text was carefully checked against old versions of the manual
- Full document is available

Maintenance

- The master LaTeX files are maintained at NNDC-BNL
- Currently M. Herman is responsible (with the support of A. Trkov from JSI, Slovenia)
- The version of the manual on the web will be kept up-to-date in accordance with CSEWG recommendations
- GFORGE system will be used for maintenance

Status

- All known updates approved by CSEWGW are included in the present version
- Some remaining typing errors reported recently are corrected and will be posted in the next CSEWGW-approved distribution
- A few suggestions for improvement are presented for CSEWGW approval (i.e. improvements and clarifications, *not* format extensions)

AJ The absolute value of AJ is the floating-point value of J (the spin, or total angular momentum, of the resonance).

When two channel spins are possible, if the sign of AJ is negative, the lower value for the channel spin is implied; if positive, the higher value is implied. When AJ is zero, only one value of channel spin is possible so there is no ambiguity; the channel spin s is equal to the orbital angular momentum l .

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Since only one of the two channel-spin widths can be specified, the other is assumed to be zero. Evaluations requiring both components to be specified should use RML formalism (LRF=7).

This convention could be used in SLBW (LRF=1) and MLBW (LRF=2), but those formalisms cannot use the information, so it is useful only in Reich-Moore (LRF=3).

The "R-Matrix Limited" (RML) format was designed to accommodate the features of R-Matrix theory as implemented in analyses codes being used for current evaluations. In this format, relevant parameters appear only once. Particle-pairs are given first: the masses, spins and parities, and charges for the two particles are specified, as well as the Q -value and the MT value (which defines whether this particle-pair represents elastic scattering, fission, inelastic, capture, etc.). Two particle-pairs will always be present: gamma + compound nucleus, and neutron + target nucleus in ground state. Other particle-pairs are included as needed.

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2.4.20 Channel Spin and Other Considerations

For the R-Matrix Limited format, channel spin is explicit and the evaluator must in general provide partial widths that depend on s as well as l and J .

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For the R-Matrix Limited format, channel spin is explicit and the evaluator must in general provide partial widths that depend on s as well as l and J . In the case of decay into inelastic channels, the above equations defining s still apply. The neutron spin is still $i = 1/2+$ (alternatively $i' = 1/2+$), J^π is still the same because it is conserved, but l' , L' and s' have nothing to do with l , L and s values in the incident channels.

1. Channel spin is effectively eliminated, because the partial widths occur in "summed" form:

$$\Gamma_{lJ} = \Gamma_{ls_1J} + \Gamma_{ls_2J} \quad (2.8)$$

Since only the sum is required, the evaluator is spared the necessity of specifying the separate s -values. This converts an (l, s, J) formalism into an (l, J) formalism. The same effect can be achieved by assuming that $I=0$, a popular assumption often made independently of the truth, as in many optical model calculations.

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Since MLBW can also describe inelastic scattering, the comment from the RML paragraph above applies: l' , L' and s' have nothing to do with the l , L , and s values in the incident channels, but note that MLBW has no explicit way to define l' , L' and s' .

Notation change request for RML (LRF=7)

- IPP (floating point number) → PPI ?
- In SAMMY the SHIFT parameter means
 - 1 = On
 - 0 = Off

In the ENDF manual SHF parameter for the same quantity means

1 = On

-1 = Off

Change convention?

For high incident energies, α and/or β values may be required that are outside the ranges tabulated for $S(\alpha, \beta)$. In these cases, the short-collision-time (SCT) approximation should be used as follows ²:

$$S^{\text{SCT}}(\alpha, \beta, T) = \frac{\exp \left[-\frac{(\alpha - |\beta|)^2 T}{4\alpha T_{\text{eff}}(T)} - \frac{|\beta|}{2} \right]}{\sqrt{4\pi\alpha \frac{T_{\text{eff}}(T)}{T}}} \quad (7.8)$$

²This equation is given correctly in the General Atomics report GA-9950, UC-80, Reactor Technology (1970), but is misprinted in LA-9303-M VOL II (ENDF-324) 1982, and in BNL-NCS-44945-05-Revised June 2005 (ENDF-102).

D.1.1.4 The Competitive Reaction Cross Section

The competitive reaction cross section, $\sigma_{n,x}(E)$, is given in terms of analogous formulas involving Γ_{cr} , the competitive width. By convention, the cross section for the competitive reaction is given entirely in File 3, and is not to be computed from the resonance parameters. The reason for this is that the latter calculation can be done correctly only for a single competitive channel, since the file can define only one competitive width.

The statistical factor $g_J = (2J + 1)/[2(2I + 1)]$ is obtained from the target spin I and the resonance spin J given in File 2 as SPI and |AJ|, respectively.

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D.1.1.5 General

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D.1.2 Multilevel Breit-Wigner (MLBW, LRF=2)

The equations are the same as SLBW, except that a resonance-resonance interference term is included in the equation for elastic scattering of l -wave neutrons, $\sigma_{n,n}^l(E)$:

$$\sigma_{n,n}^l(E) = \frac{\pi}{k^2} \sum_J g_J \sum_{r=2}^{\text{NR}_J} \sum_{s=1}^{r-1} \frac{2\Gamma_{nr}\Gamma_{ns} [(E - E'_r)(E - E'_s) + \frac{1}{4}\Gamma_r\Gamma_s]}{[(E - E'_r)^2 + (\Gamma_r/2)^2] [(E - E'_s)^2 + (\Gamma_s/2)^2]} \quad (\text{D.15})$$

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$$\begin{aligned} \sigma_{n,n}^l(E) &= (2l + 1) \frac{4\pi}{k^2} \sin^2 \phi_l \quad (\text{D.15}) \\ &+ \frac{\pi}{k^2} \sum_J g_J \sum_{r=1}^{\text{NR}_J} \frac{\Gamma_{nr}^2 - 2\Gamma_{nr}\Gamma_r \sin^2 \phi_l + 2(E - E'_r) \Gamma_{nr} \sin(2\phi_l)}{(E - E'_r)^2 + \frac{1}{4}\Gamma_r^2} \\ &+ \frac{\pi}{k^2} \sum_J g_J \sum_{r=2}^{\text{NR}_J} \sum_{t=1}^{r-1} \frac{2\Gamma_{nr}\Gamma_{nt} [(E - E'_r)(E - E'_t) + \frac{1}{4}\Gamma_r\Gamma_t]}{[(E - E'_r)^2 + (\Gamma_r/2)^2] [(E - E'_t)^2 + (\Gamma_t/2)^2]} \end{aligned}$$

where

$$G_r = \frac{1}{2} \sum_{s=1, s \neq r}^{NR_J} \frac{\Gamma_{nr} \Gamma_{ns} (\Gamma_r + \Gamma_s)}{(E'_r - E'_s)^2 + \frac{1}{4} (\Gamma_r + \Gamma_s)^2}, \quad (\text{D.17})$$

$$H_r = \sum_{s=1, s \neq r}^{NR_J} \frac{\Gamma_{nr} \Gamma_{ns} (E'_r - E'_s)}{(E'_r - E'_s)^2 + \frac{1}{4} (\Gamma_r + \Gamma_s)^2} \quad (\text{D.18})$$

For the user who does not require ψ - and χ -broadening, the amplitude-squared form of the equations, which are mathematically identical to the conventional MLBW equations, require less computing time

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$$H_r = \sum_{t=1, t \neq r}^{NR_J} \frac{\Gamma_{nr} \Gamma_{nt} (E'_r - E'_t)}{(E'_r - E'_t)^2 + \frac{1}{4} (\Gamma_r + \Gamma_t)^2} \quad (\text{D.19})$$

For applications that do not require ψ - and χ -Doppler broadening, the amplitude-squared form of the equations, which are mathematically identical to the conventional MLBW equations, require less computing time

Format extensions

- A few additional proposals were circulated by Cecil Lubitz
- They represent format extensions, which need to be applied/tested on practical examples by the interested parties
- So far the available information is not sufficient for inclusion in the manual

Conclusion

- Conversion of the manual into LaTeX was successfully completed
- The manual is up-to-date with CSEWG-approved extensions
- Simpler maintenance will help to reduce errors
- **Your feedback? Help us to help you!**
(Cecil, thank you!)